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KINETICS OF CONDENSATION
FROM THE VAPOR PHASE

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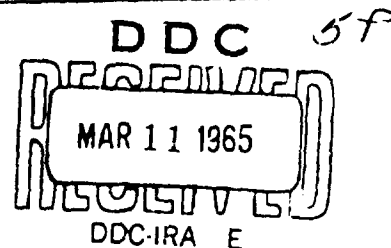
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I. SUMMARY

The theoretical problems involved in nucleation are being re-examined further. Theoretical computation of cluster energy using a simple molecular-pair model is currently being explored.

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II. INTRODUCTION

This program is a fundamental investigation of the kinetics and mechanisms of condensation and particularly of homogeneous nucleation from the vapor phase.

This report is the third quarterly report of the one year extension to Contract NONr 4154(00).

In our opinion, the current situation in condensation kinetics is that good experimental data on water condensation is available (cloud chamber, shock tube, and perhaps wind tunnel data) but no satisfactory theory of nucleation is available.

Therefore, during the past quarter we have been re-examining the theoretical problems in nucleation once again.

III. PRESENT WORK

Clusters which contain 50 or so molecules seem to be the ones of interest in nucleation.

The problem is to predict the thermodynamic equilibrium concentration of such clusters. This equilibrium concentration of a certain sized cluster is related to the free energy of the cluster. The free energy of the cluster in turn involves its translation and rotation energies (as noted by Lothe and Pound) and also the vibration energy of the cluster.

There appear to be two general approaches to the vibration-energy problem. The conventional approach is to separate the vibration energy of the cluster into surface and volume energies. The classical theory uses macroscopic surface and volume energies. Numerous people have of course questioned the validity of using the macroscopic surface energy for the small clusters of interest here.

The remaining problem using this approach is to determine the relationship between the volume energy of the g molecules in the cluster and the volume energy of g molecules in the bulk condensed phase. That is, the bulk condensed phase is convenient to use as a reference state, but the relation between the cluster vibrations and the bulk vibrations remains obscure.

For example, in our opinion, Kuhrt correctly evaluates the relationship between surface and volume vibrations but incorrectly assumes that the volume vibrations in a cluster are identical to the volume vibrations in the bulk

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condensed phase.

Thus, some of the energy of a molecule in the bulk condensed phase arises from an interaction with distant atoms because of the long range van der Waal forces. Obviously, these long-range energies cannot occur in a small cluster. The question thus arises as to a quantitative theory for indicating precisely how important they are. That is, the long-range energies do not contribute to the cluster energy, and referring the cluster energy to bulk energy results in an overestimate of the stability of the cluster.

The entire problem of cluster thermodynamics could be resolved if the Mayer-type cluster integral were satisfactorily resolved for various cluster sizes and for various materials of interest. We are presently following this last approach, using a simple molecular pair interaction model.

At present, we are (1) revising our manuscript titled "Re Examination of Nucleation and Condensation of Water" and (2) using a computer to evaluate the energies of various sized argon clusters. A detailed summary of the computation of cluster energy will be given in the next report.

Interpretation of the experimental data must wait until the above work is at least semi-quantitatively completed.